Automated structure based classification of crude oil samples with 2D-HMBC NMR spectra

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Crude oils are complex mixtures of organic compounds that can be studied by a number of physicochemical methods including NMR[1, 2]. The 1D proton NMR spectrum has been frequently used to characterize these samples since it provides a general and quantitative characterization of the sample composition[1, 2]. The application of 2D ^{1}H-^{13}C NMR correlation experiments to these samples has not been used extensively. Despite its lower sensitivity and longer acquisition time required than 1D proton spectrum, the enhanced signal dispersion provided by these 2D NMR experiments may reveal fine structural details related of the most abundant components in the crude-oil. Thus, these experiments could provide a basis for crude oil classification on the assumption that similar spectra indicate similar chemical structures.

We have developed a generic software tool for the automatic analysis and comparison of multidimensional NMR data sets. The classification algorithm introduced consisted in four stages that are applied sequentially i) spectral bucketing integration, ii) similarity matrix calculations, iii) Principal Component Analysis (PCA) and iv) k-means cluster analysis.

We have applied this classification protocol to 58 crude oils samples of different origins that were analyzed with 2D-HMBC spectra. The results showed that this classification method is able to discern subtle differences in the composition of the crude-oils, and interestingly enough it was found to be sensitive to crude-oil sample evolution during time.

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